Acetone

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -87.6 °C

Global applicability domain: Inside

Local applicability domain index: 8.17e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

Image not found
Acetone
Measured: -96.6
Predicted: -87.6

Image not found
(2H6)Acetone
Measured: -96.6
Predicted: -87.6

Image not found
Propanal
Measured: -80.0
Predicted: -86.0

Image not found
Methyl ethyl ketone
Measured: -86.6
Predicted: -78.1

Image not found
Butyraldehyde
Measured: -99.0
Predicted: -85.8

Image not found
2-Methylpropanal
Measured: -65.9
Predicted: -55.3